Final Report

Annual Application of MM5 to Support 1994 Calpuff Air Quality Modeling

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1 INTRODUCTION

This document presents the application methodology and evaluation results of an annual mesoscale meteorological modeling in support of air quality assessments.

1.1 Background

Over the past half decade, emergent requirements for direct numerical simulation of urban and regional scale photochemical and secondary aerosol air quality—spawned largely by the new particulate matter ($PM_{2.5}$) and regional haze regulations—have led to intensified efforts to construct high-resolution emissions, meteorological and air quality data sets. The concomitant increase in computational throughput of low-cost modern scientific workstations has ushered in a new era of regional air quality modeling. It is now possible, for example, to exercise sophisticated mesoscale prognostic meteorological models and Eulerian and Lagrangian photochemical/aerosol models for the full annual period, simulating ozone, sulfate and nitrate deposition, and secondary organic aerosols (SOA) across the entire United States (U.S.) or over discrete subregions.

1.2 Study objectives

Consistent with ongoing U.S. Environmental Protection Agency (EPA) programs, this work assignment is aimed at developing gridded meteorological data sets that can be used to support regional scale air quality modeling of SO2 sources in the vicinity of the Fort Pack Indian Reservation and Medicine Lake Wilderness Area in eastern Montana and the Theodore Roosevelt National Park and Lostwood Wilderness area in western North Dakota.

2 METHODOLOGY

The methodology for this approach is very straightforward. The MM5 model is applied to calendar 1994 and the model results are compared with available observations and synoptic weather charts.

2.1 Model Selection and Application

Below we give a brief summary of the MM5 input data preparation procedures we propose for the episodic and annual modeling exercises.

<u>Model Selection</u>: The most recent version of the publicly available non-hydrostatic version of MM5 (version 3.5) is used. The MM5 released terrain, pregrid, little_r and interpf processors were used to develop model inputs.

<u>Horizontal Domain Definition:</u> The computational region is presented in Figure 2-1. The projection is Lambert Conformal with the "national RPO" grid projection pole of 40^0, -97^0 with true latitudes of 33^0 and 45^0.

Vertical Domain Definition: The MM5 modeling is based on 35 vertical layers with an approximately 50 meter deep surface layer. The MM5 vertical domain is presented in both sigma and height coordinates in Table 2-1.

Topographic Inputs: Topographic information for the MM5 is developed using the NCAR and the United States Geological Survey (USGS) terrain databases. The 180 and 60 km grids are based the 10 min (~18 km) Geophysical Data Center global data. The 20 km grid is based on the 5 min (~9 km) Geophysical Data Center global data. Terrain data is interpolated to the model grid using a Cressman-type objective analysis scheme. To avoid interpolating elevated terrain over water, after the terrain databases are interpolated onto the MM5 grid, the NCAR graphic water body database was used to correct elevations over water bodies.

Vegetation Type and Land Use Inputs: Vegetation type and land use information is developed using the most recently released NCAR/PSU databases provided with the MM5 distribution. The 108 and 36 km grids use the 2 min. (~ 4 km). Standard MM5 surface characteristics corresponding to each land use category will be employed.

Atmospheric Data Inputs: The first guess atmosphere data are extracted from the NCAR/NCEP Reanalysis Project (NNRP) archives. Surface and upper-air observations used in the objective analyses, following the procedures outlined by Stauffer and Seaman at PSU, are quality-inspected by MM5 pre-processors using automated gross-error checks and "buddy" checks. In addition, rawinsonde soundings undergo vertical consistency checks. The synoptic-scale data used for this initialization (and in the analysis nudging discussed below) are obtained from the conventional National Weather Service (NWS) twice-daily radiosondes and 3-hr NWS surface observations.

Water Temperature Inputs: The NNRP contains a “skin temperature” field. This can be used as a water temperature input to MM5. It is recognized that these skin temperatures can lead to temperature errors along coastlines. However, for this sort of analysis focusing on bulk continental scale transport, this issue is likely not important.

FDDA Data Assimilation: This simulation uses an analysis-nudging technique where the observations are nudged toward a field prepared by objectively analyzing surface and aloft monitor data into the first-guess fields. For these simulations a nudging coefficient of $2.5x10^{-4}$ was used for winds and temperature and $1x10^{-5}$ for mixing ratio. Only 3D analysis nudging was performed and thermodynamic variables are not nudged within the boundary layer.

Physics Options: The MM5 model physics options in this simulation are as follows:

Kain-Fritsch Cumulus Parameterization
Blackadar PBL Scheme
Simple Ice Moisture Scheme
RRTM Atmospheric Radiation Scheme

Multi-layer Soil Temperature Model

2.2 Evaluation Approach

The model evaluation approach is based on a combination of qualitative and quantitative analyses. The qualitative approach is to compare hourly temperature, mixing ratio, and wind vector plots with observations over a range of data. The statistical approach is to examine the model bias and error for temperature, mixing ratio and the index of agreement for the windfields.

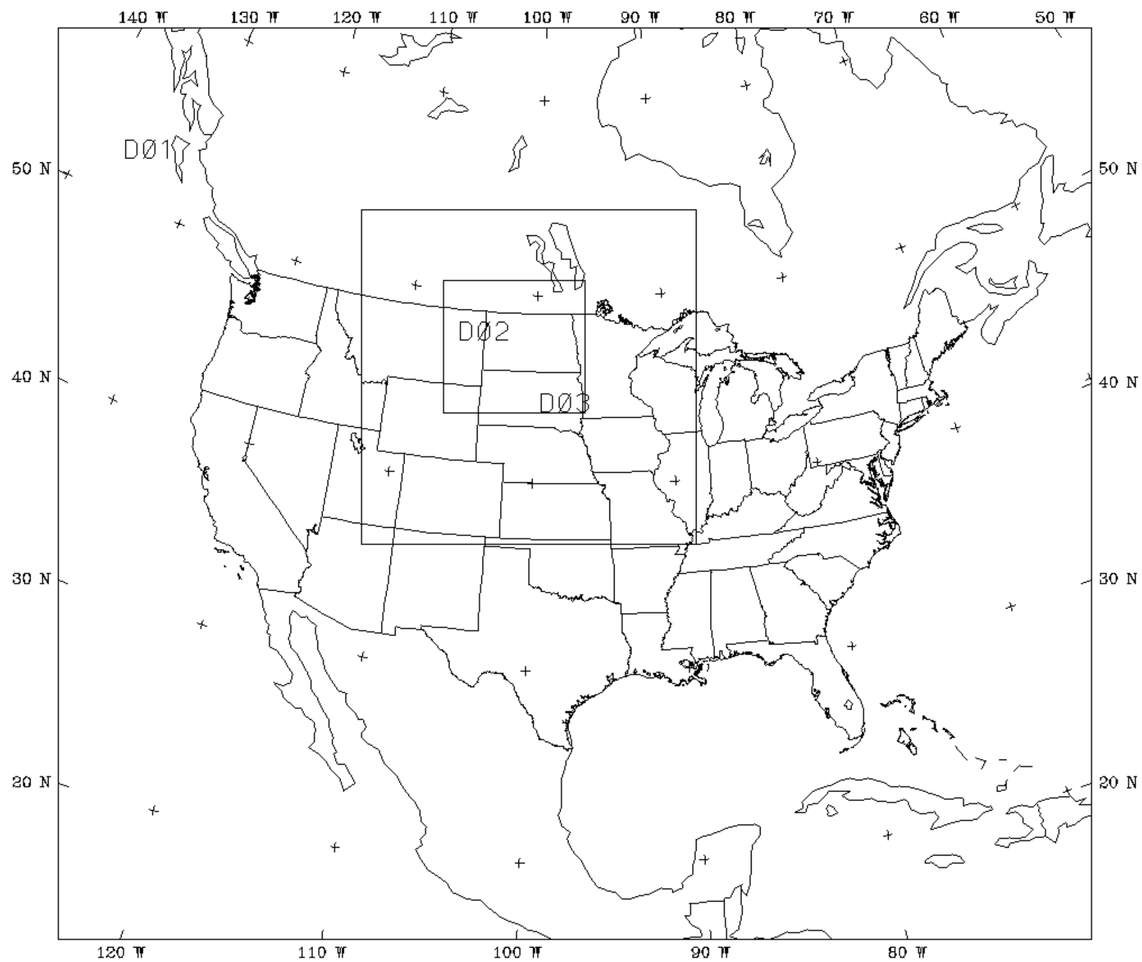
Interpretation of bulk statistics over a region the size of that covered by the 20 km domain is problematic. It is difficult to detect if the model is missing important sub-regional features.

The observed database for winds, temperature, and water mixing ratio used in this analysis is the NOAA Techniques Development Lab (TDL) Surface Hourly Observation database obtained from the NCAR archives. The rain observations are taken from the National Climatic Data Center (NCDC) 3240 hourly rainfall archives.

Table 2-1: MM5 Vertical Domain Specification.

k(MM5)	sigma	press.(mb)	height(m)	depth(m)
35	0.0000	10000	15674	2004
34	0.0500	14500	13670	1585
33	0.1000	19000	12085	1321
32	0.1500	23500	10764	1139
31	0.2000	28000	9625	1004
30	0.2500	32500	8621	900
29	0.3000	37000	7720	817
28	0.3500	41500	6903	750
27	0.4000	46000	6153	693
26	0.4500	50500	5461	645
25	0.5000	55000	4816	604
24	0.5500	59500	4212	568
23	0.6000	64000	3644	536
22	0.6500	68500	3108	508
21	0.7000	73000	2600	388
20	0.7400	76600	2212	282
19	0.7700	79300	1930	274
18	0.8000	82000	1657	178
17	0.8200	83800	1478	175
16	0.8400	85600	1303	172
15	0.8600	87400	1130	169
14	0.8800	89200	961	167
13	0.9000	91000	794	82
12	0.9100	91900	712	82
11	0.9200	92800	631	81
10	0.9300	93700	550	80
9	0.9400	94600	469	80
8	0.9500	95500	389	79
7	0.9600	96400	310	78
6	0.9700	97300	232	78
5	0.9800	98200	154	39
4	0.9850	98650	115	39
3	0.9900	99100	77	38
2	0.9950	99550	38	38
1	0.9975	99775	19	19
0	1.0000	100000	0	0

Figure 2-1: Nested Computational Grid. (D01 is at 180km, D02 is at 60km and D03 is at 20km)



3 RESULTS

The synoptic and statistical evaluations for the episode are presented in the following sections.

3.1 Qualitative Evaluation

The qualitative evaluation involved plotting surface wind vectors, temperature, mixing ratio, and monthly total precipitation plots with observations overlayed on the model predictions. Aloft comparsions included skew-T log P plots for all available soundings. Space precludes inclusion of the graphics in this report, but hourly results are presented on the accompanying CD. Sample plots for temperature, mixing ratio, wind vector, annual precipitaion and skew-T log P plots are presented in Figure 3-1 through 3-5, respectively.

3.2 Statistical Evaluation

The results for the statistical evaluation are presented in this section. Summary statistics for temperature, mixing ratio, wind index of agreement and monthly total precipitation are presented in Table 3-1. A comparison table of other MM5 modeling studies is presented in Table 3-2. When comparing the modeling results it is important to remember that the majority of the simulations presented in Table 3-2 were for episodic (i.e. approximately one to two weeks) episodes performed at 12km horizontal spacing.

Temperature bias and error are presented in Table 3-1. The model is slightly too warm January through August and slightly too cool September through December. Averaged over the entire year the model bias is a positive 0.28 deg. C. The temperature bias and errors are well within the range of values for the 40 MM5 applications summarized in Table 3-2. Mean temperature values for both observations and the model estimates at the observation locations are presented in Figures 3-6 through 3-8. The model is able to capture both the annual temperature trend and more synoptic (ie few day timescales) events quite accurately.

The mixing ratio summary bias and error data in Table 3-1 shows that the model is somewhat too dry in the summer months and somewhat too moist in the spring, fall and winter. The overall annual average bias and error agree well with other MM5 applications, and the model error (1.03 g/kg) is less than the historical average of 2.0. Mean mixing ratio for both observations and the model estimates at the observation locations are presented in Figures 3-9 through 3-11. Overall the mixing ratio trends are accurately replicated except the model tends to overestimate mixing ratio for certain periods. The model overestimating precipitation events likely causes this.

To summarize the wind performance a metric known as Index of Agreement (IA) is used. IA is defined as:

$$I = 1 - \left[\frac{N\ (RMSE)^{2}}{\sum_{i=1}^{N} \left(\left| \Phi_{ei} - M_{o} \right| + \left| \Phi_{oi} - M_{o} \right| \right)^{2}} \right]$$

where:

N is the number of observations that hour
RMSE is the root mean squared error
Ö_{ei} represents the model predictions at station i
Ö_{oi} represents the observations at station i
Mo is the mean observation at that hour

This metric condenses all the differences between model estimates and observations into one statistical quantity. It is the ratio of the cumulative difference between the model estimates and the corresponding observations to the sum of two differences: between the estimates and observed mean and the observations and the observed mean. Viewed from another perspective, the index of agreement is a measure of how well the model estimates departure from the observed mean matches, case by case, the observations' departure from the observed mean. Thus, the correspondence between estimated and observed values across the domain at a given time may be quantified in a single metric and displayed as a time series. The index of agreement has a theoretical range of 0 to 1, the latter score suggesting perfect agreement.

Wind index of agreement is consistent throughout the year at approximately 0.7. This is approximately the same as the average of the historical MM5 simulations of 0.69. Time series plots of the index of agreement are presented in Figures 3-12 through 3-14. The index of agreement plots show fairly large variability with no clear annual trends.

Monthly total rainfall bias and errors are summarized in Table 3-1. The monthly rainfall totals are computed by summing all the observed rainfall and all the model predicted rainfall at the grid cells where rainfall monitors are located. Overall the model is tending to overestimate rainfall in January through April and to underestimate for the remainder of the year. This trend is very clearly presented in Figure 3-15. The largest model mean estimation error is approximately 3 cm. in October.

Table 3-1: Performance Metrics for 20km 1994 Annual MM5 Simulation.

Metric	Jan-Apr	May-Aug	Sep-Dec	Annual
Mixing Ratio Bias (g/kg)	0.53	-0.43	0.35	0.15
Mixing Ratio Error (g/kg)	0.67	1.60	0.81	1.03
Temperature Bias (K)	1.06	0.40	-0.61	0.28
Temperature Error (K)	3.05	1.91	2.49	2.48
Wind Index of Agreement	0.71	0.73	0.72	0.72
Precipitation Bias (cm)	1.05	-1.07	-0.58	-0.20
Precipitation Error (cm)	1.27	2.91	1.69	1.96

Table 3-2: **Summary of Alpine Geophysics Regional Prognostic Meteorological Model Performance Evaluations Since 1995.**

No	Study	Domain	Model	Ref	Episode	Temperature, (deg C)		Mix Ratio, (gm/Kg)			Surface Winds (m/s)		
						Bias	Error	Bias	Error	Error	RMSE	Indx A	Wdir Dif
1	DAQM	Rocky Mtns	MM5	13	12-20 Jan '97	0.5	1.7			52.2	2.52	0.66	65
2	DAQM	Rocky Mtns	MM5	13	28-30 Dec '87	0.3	1.6			-5.2	2.76	0.71	2
3	SAMI	SE U.S.	RAMS	7	24-29 May '95	-1.0	1.9	0.0	0.8	35.0	1.90	0.76	13
4	SAMI	SE U.S.	RAMS	7	11-17 May '93	-1.5	2.1	0.0	0.8	51.0	1.90	0.76	6
5	SAMI	SE U.S.	RAMS	7	23-31 Mar '93	-1.3	2.2	0.0	0.6	53.0	2.27	0.74	100
6	SAMI	SE U.S.	RAMS	7	8-13 Feb '94	0.5	2.1	0.0	0.4	63.0	2.76	0.72	103
7	SAMI	SE U.S.	RAMS	7	3-12 Aug '93	-0.4	1.6	-0.6	1.1	140.0	2.18	0.75	25
8	SAMI	SE U.S.	RAMS	7	22-29 Jun '92	-1.1	1.8	0.0	1.0	66.0	1.89	0.75	20
9	SAMI	SE U.S.	RAMS	7	24Ap-3My '91	-0.8	1.8	-0.1	0.7	60.0	2.35	0.81	4
10	COAST '93	Cent. U.S.	MM5	11	4-11 Sept '93	0.2	1.8	0.1	1.4	61.4	2.20	0.69	15
11	COAST '93	Cent. U.S.	MM5	12	6-11 Sept '93	-0.3	1.9	2.4	12.8	50.0	1.77	0.55	65
12	COAST '93	Cent. U.S.	RAMS	12	6-11 Sept '93	-0.5	2.4	3.6	8.6	10.2	1.12	0.57	82
14	TexAQS2000	Cent. U. S.	MM5-T	12	25Ag-1 Sp '00	0.2	1.6	-0.5	1.9	13.2	1.88	0.61	14
15	TexAQS2000	Cent. U. S.	MM5-M	12	25Ag-1 Sp '00	-0.4	2.0	0.2	2.3	19.5	1.96	0.44	27
16	PFOS	SE U.S.	MM5	10	16-24 Apr '99	0.1	1.5	-0.1	1.2	20.9	1.94	0.78	10
17	PFOS	SE U.S.	MM5	10	2-10 May '97	0.2	1.6	0.1	1.2	21.0	1.95	0.78	32
18	PFOS	SE U.S.	MM5	10	25-30 Aug '97	0.2	1.7	-2.0	2.3	30.6	1.86	0.73	32
19	PFOS	SE U.S.	MM5	10	4-10 Apr '99	-0.4	1.3	0.8	1.5	18.1	1.80	0.80	8
20	PFOS	SE U.S.	MM5	10	17-23 Sep '97	0.1	1.6	-0.4	1.6	27.9	1.84	0.72	9
21	PFOS	SE U.S.	MM5	10	25-28 Aug '98	0.2	1.5	0.9	1.8	51.2	1.76	0.78	32
22	PFOS	SE U.S.	MM5	10	8-10 May '99	0.2	2.2	0.3	1.4	49.8	1.69	0.77	19
26	MoKAN	Midwest U.S.	MM5	8	8-15 Jul '95	0.2	1.7	-0.6	1.6	10.3	1.86	0.41	1
27	MoKAN	Midwest U.S.	MM5	8	14-21 Aug '98	2.0	2.3	2.4	2.6	47.5	1.83	0.45	4
28	MoKAN	Midwest U.S.	MM5	8	11-24 Jun '95	-0.3	1.6	-0.9	1.3	31.6	1.88	0.48	20
29	Pittsbrg SIP	East U.S.	MM5	1	31Jy-2 Ag '95	0.8	2.4	0.2	2.2	12.6	1.78	0.75	8
30	SARMAP	West U.S.	MM5	4	3-6 Aug '90	0.2	2.9	-0.2	1.9	22.6	2.13	0.80	3
31	CRC-LMOS	Midwest U.S.	RAMS	6	26-28 June '91	0.1	1.4	-0.1	1.2	11.9	1.82	0.69	17
32	CRC-LMOS	Midwest U.S.	RAMS	6	17-19 Jul '91	0.0	1.9	0.4	1.4	3.5	1.73	0.64	7
33	CRC-LMOS	Midwest U.S.	MM5	6	26-28 Jul '91	-0.5	1.6	-0.1	1.2	5.8	1.70	0.79	14
34	CRC-LMOS	Midwest U.S.	MM5	6	17-19 Jun '91	-0.3	1.7	-0.6	1.5	15.6	1.65	0.77	7

35	OTAG	East U.S.	RAMS	3	13-21 Jul '91	1.6	2.1	0.0	1.2	4.6	1.61	0.74	27
36	OTAG	East U.S.	MM5	3	13-21 Jul '91	-0.1	2.0	-0.3	1.4	23.0	1.92	0.73	17
37	OTAG	East U.S.	MM5	2	1-11 Jul '88	-0.6	3.3	-1.4	2.0	65.6	3.21	0.64	8
38	OTAG	East U.S.	MM5	1	12-15 Jul '95	-0.2	2.0	-1.5	2.2	21.2	1.91	0.68	15
39	Cincy SIP	Midwest U.S.	MM5	5	18-22 Jun '94	-0.7	2.4	-1.6	2.2	82.4	2.69	0.80	0
40	BAMP	SE U.S.	MM5	9	6-11 Sept '93	-0.4	2.1	-0.6	1.0	89.4	2.36	0.60	22
	Mean					-0.1	1.9	0.0	2.0	37.9	1.97	0.69	23

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Figure 3-1: Surface (10m) Temperature (Deg. C) at 1800 GMT 25 May 1994. Numbers Denote Observations.

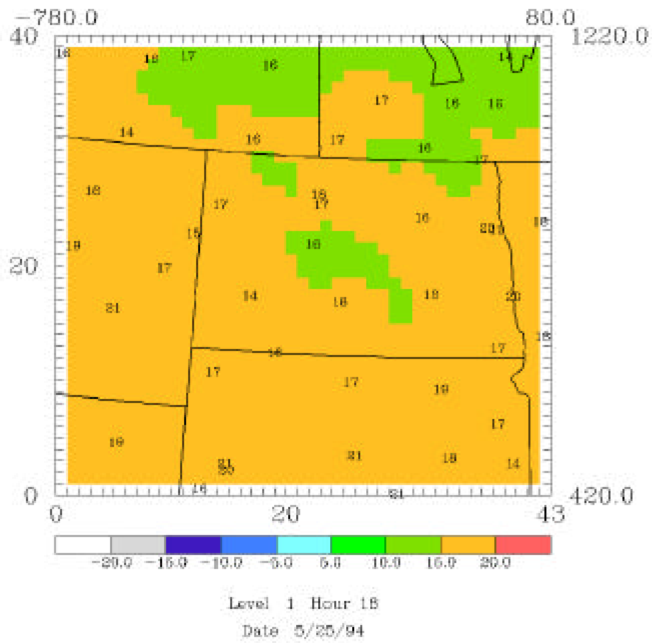


Figure 3-2: Surface (10m) Mixing Ratio (g/kg) at 1800 GMT 25 May 1994. Numbers Denote Observations.

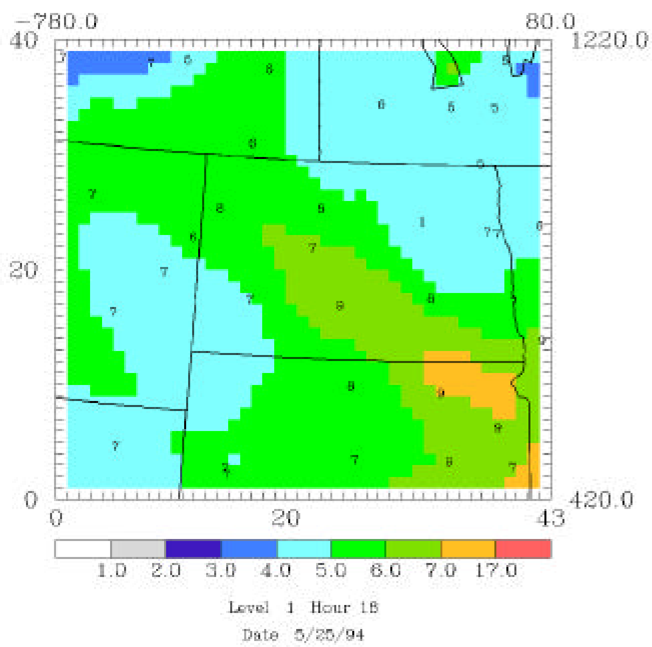


Figure 3-3: Surface (10m) Wind Vector Plot of 1800 GMT 25 May 1994. Red Vectors Denote Observations.

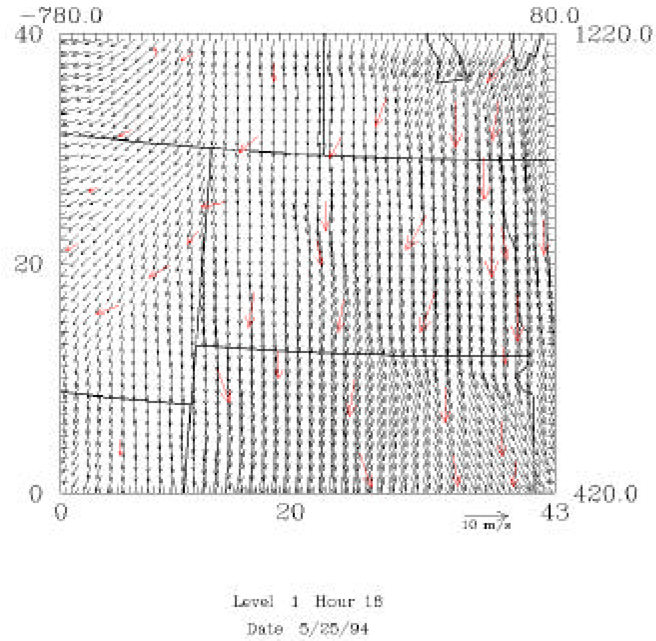


Figure 3-4: Skew-T log P plot for Bismarck ND on 25 May 1994 at 1200 GMT. Red is Observed and Blue is Model Predicted.

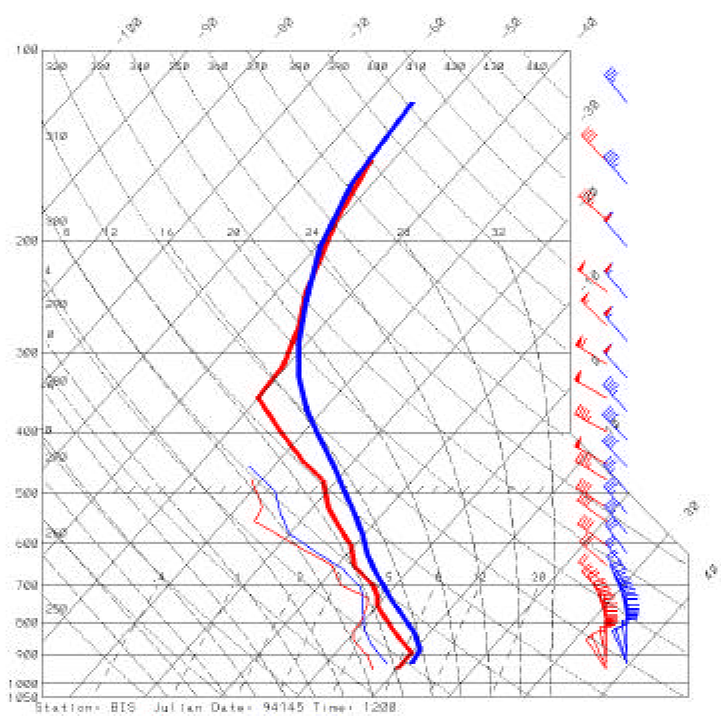


Figure 3-5: Annual Total Preciptation (cm). for 1994. Numbers Denote Observations.

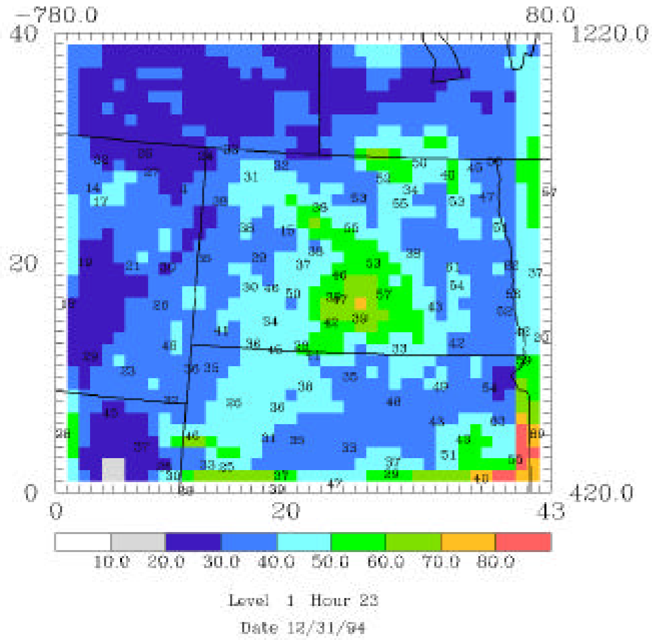


Figure 3-6: Spatial Mean Temperature for January through April 1994 over the 20km Domain.

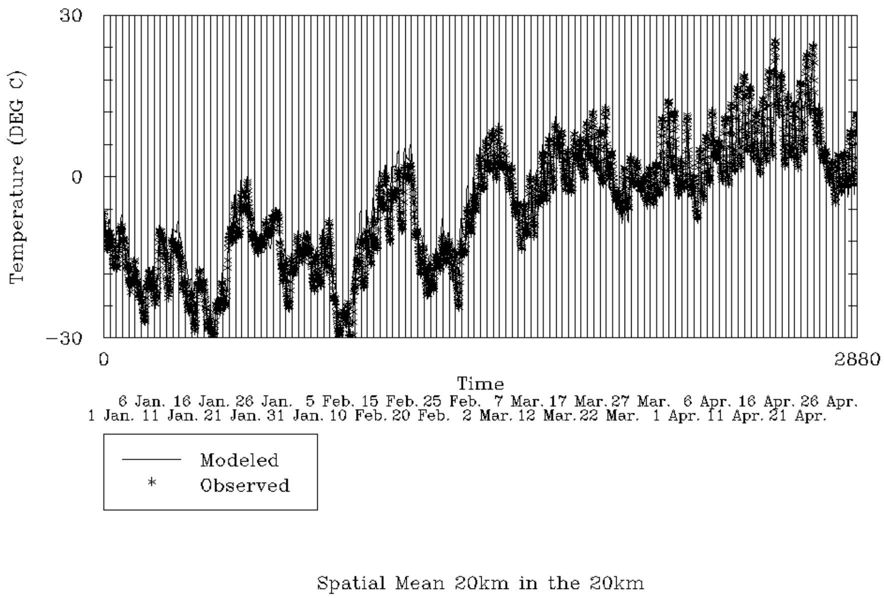


Figure 3-7: Spatial Mean Temperature for May through August 1994 over the 20km Domain.

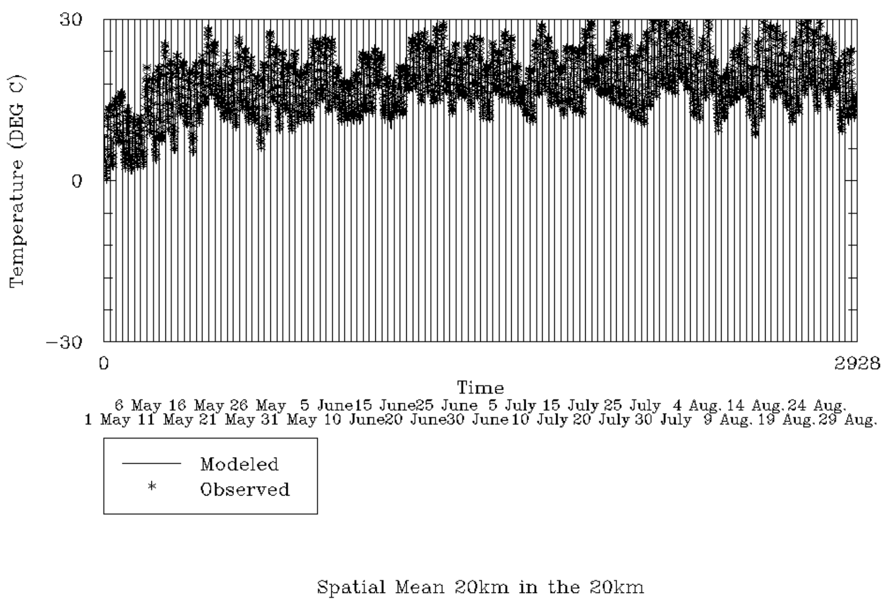


Figure 3-8: Spatial Mean Temperature for September through December 1994 over the 20km Domain.

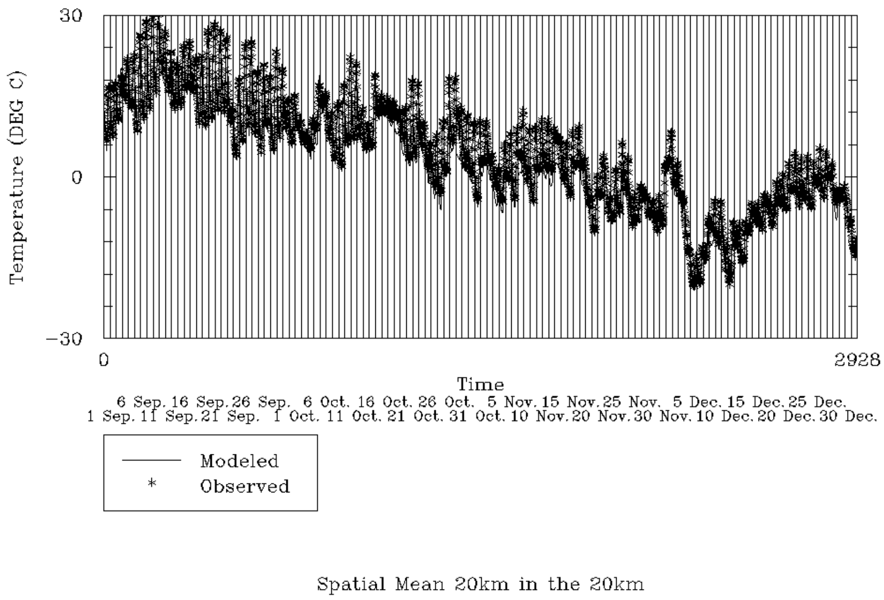


Figure 3-9: Spatial Mean Mixing Ratio (g/kg) for January through April 1994 over the 20km Domain.

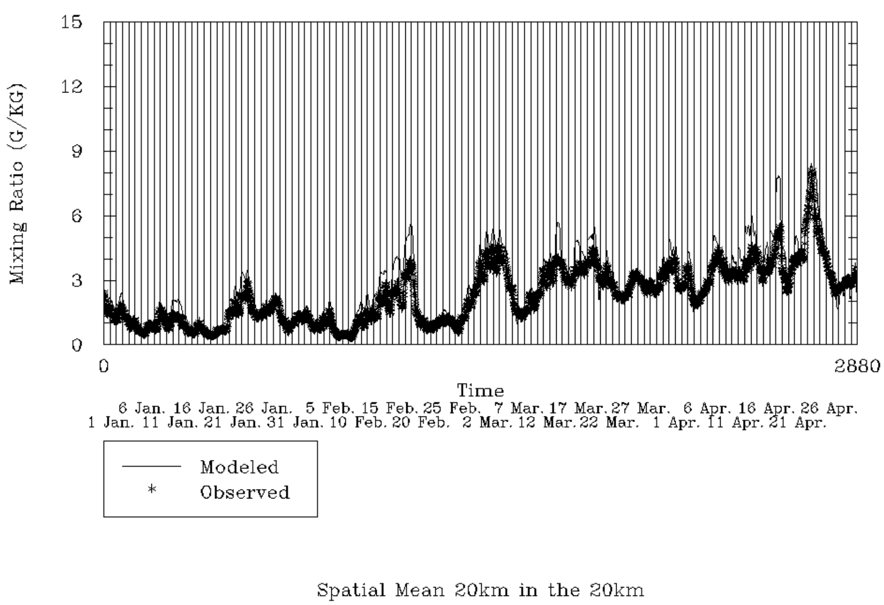


Figure 3-10: Spatial Mean Mixing Ratio (g/kg) for May through August 1994 over the 20km Domain.

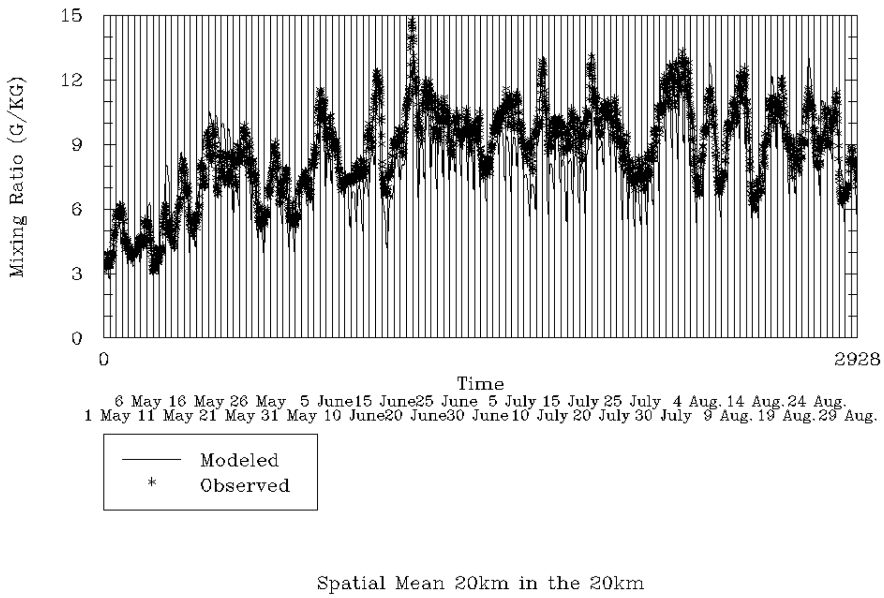


Figure 3-11: Spatial Mean Mixing Ratio (g/kg) for September through December 1994 over the 20km Domain.

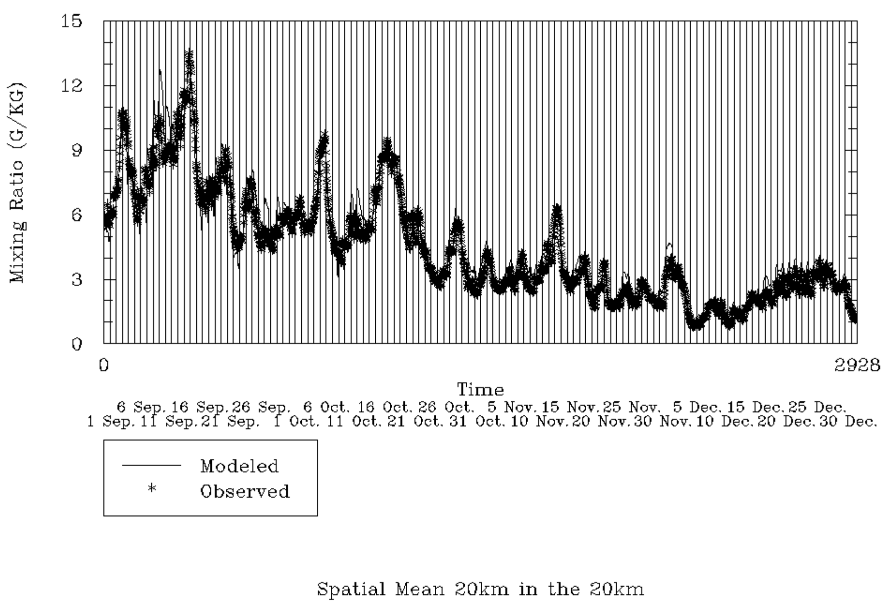


Figure 3-12: Index of Agreement for January through April 1994 over the 20km Domain.

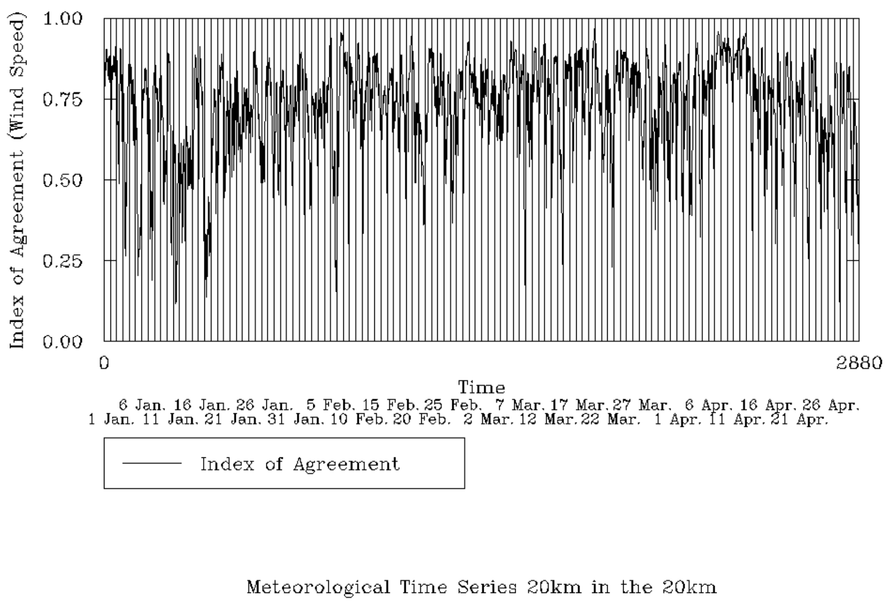


Figure 3-13: Index of Agreement for May through August 1994 over the 20km Domain.

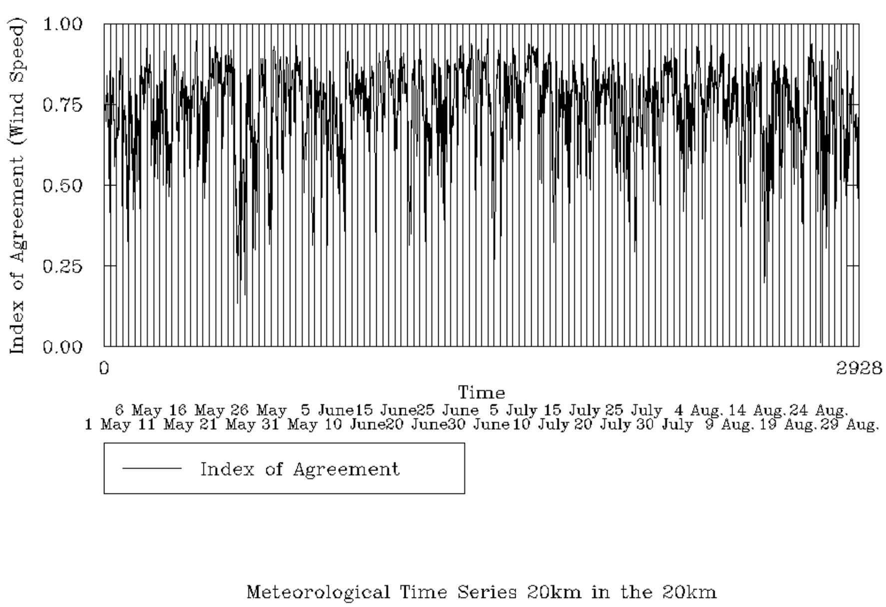


Figure 3-14: Index of Agreement for September through December 1994 over the 20km Domain.

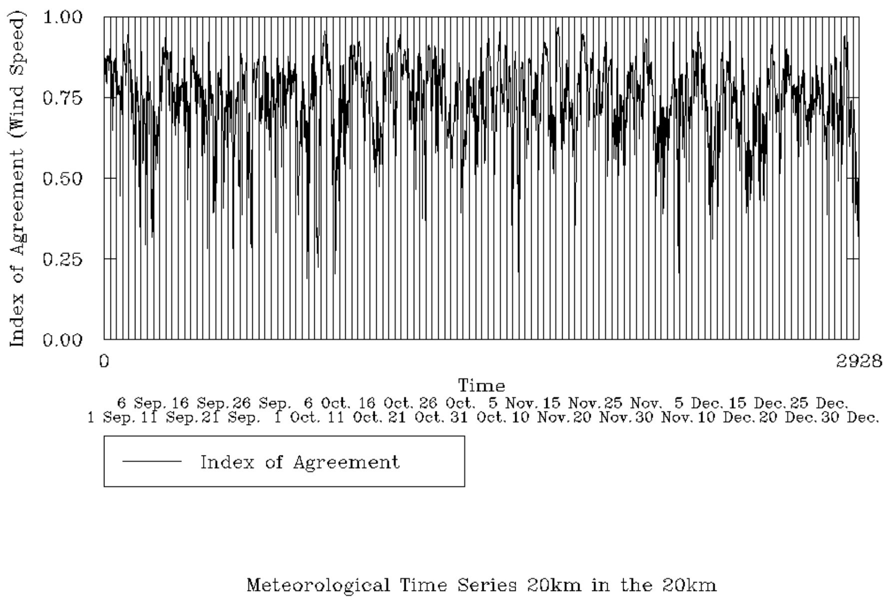
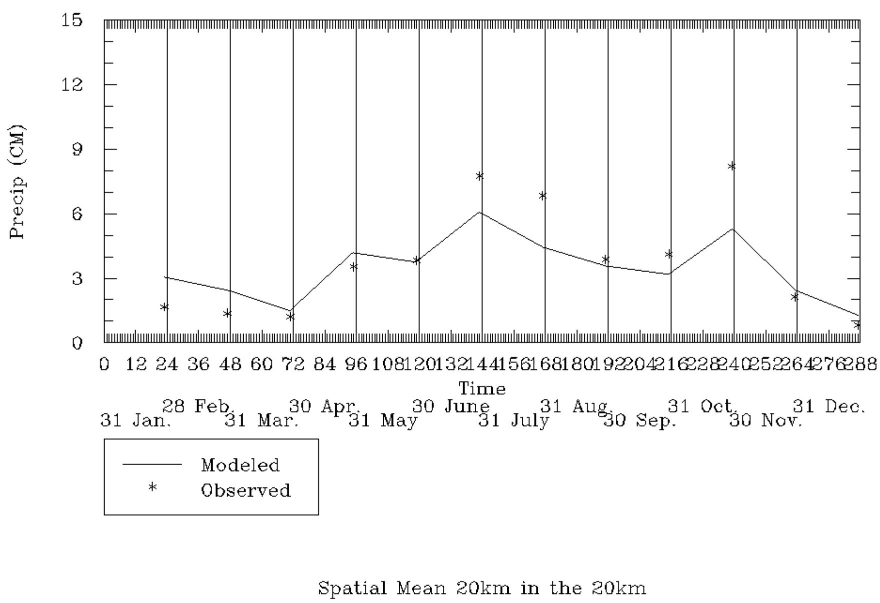


Figure 3-15: Spatial Mean Monthly Total Precipitation (cm)



4 DISCUSSION

The MM5 model has been applied in a 180/60/20km nested mode to examine flow patterns in Eastern Montana, North Dakota, and South Dakota. The model results have been analyzed against routinely available surface temperature, mixing ratio, winds and precipitation data. When compared with 40 historic MM5 applications, the model is operating with approximately the same skill level. Many of the historic MM5 applications were performed in support of State Implementation Plan (SIP) photochemical modeling studies and were found acceptable for use in regulatory modeling. The author sees no reason the model results should not be used for regional air quality modeling purposes.